

March 8, 2012

**Ozone-temperature diurnal and longer term correlations, in the lower thermosphere, mesosphere and stratosphere, based on measurements from SABER on TIMED**

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**Abstract.** The analysis of mutual ozone-temperature variations can provide useful information on their interdependencies relative to the photochemistry and dynamics governing their behavior. Previous studies have mostly been based on satellite measurements taken at a fixed local time in the stratosphere and lower mesosphere. For these data, it is shown that the zonal mean ozone amounts and temperatures in the lower stratosphere are mostly positively correlated, while they are mostly negatively correlated in the upper stratosphere and in the lower mesosphere. The negative correlation, due to the dependence of photochemical reaction rates on temperature, indicates that ozone photochemistry is more important than dynamics in determining the ozone amounts. In this study, we provide new results by extending the analysis to include diurnal variations over 24 hrs of local time, and to larger spatial regimes, to include the upper mesosphere and lower thermosphere (MLT). The results are based on measurements by the SABER instrument on the TIMED satellite. For mean variations (i.e., averages over local time and longitude) in the MLT, our results show that there is a sharp reversal in the correlation near 80 km altitude, above which the ozone mixing ratio and temperature are mostly positively correlated, while they are mostly negatively correlated below 80 km. This is consistent with the view that above ~80 km, effects due to dynamics are more important compared to photochemistry. For diurnal variations, both the ozone and temperature show phase progressions in local time, as a function of altitude and latitude. For temperature, the phase progression is as expected, as they represent migrating tides. For day time ozone, we also find regular phase progression in local time over the whole altitude range of our analysis, 25 to 105 km, at least for low latitudes. This was not previously known, although phase progressions had been noted by us and by others at lower altitudes. For diurnal variations, we find that between about 40 and 65 km, the ozone amounts and temperatures are mostly negatively correlated or neutral, while below ~40 km they are mostly positively correlated or neutral. The correlations are less systematic and less robust than for correlations of the mean. At altitudes above ~65 km, the correlations are more complex, and depend on the tidal temperature variations. For the diurnal case, consideration needs to be given to transport by thermal tides and to the efficacy of response times of ozone concentrations and temperature to each other.

## 1.0 Introduction

Because of the interdependency of ozone amounts and temperature, comparisons of their mutual variations can provide useful information on both the temperature-dependent photochemical reaction rates and the relative importance of photochemistry versus dynamics in determining the ozone concentration. Dynamics can be important not just for the transport of ozone, but for other species that play a role in the photochemistry involving ozone. For example, depending on the altitude and latitude, chemical lifetimes of odd oxygen, ( $O + O_3$ ), can vary from less than minutes

to weeks or longer. The time scales for transport by atmosphere dynamics can also vary over a large time span, for thermal diurnal tides on one hand, and large scale circulation on the other.

In the following, we present new results for a) diurnal variations over 24 hrs local time from 25 to 105 km, and b) extend the results for mean variations to higher altitudes in the mesosphere and lower thermosphere, up to 105 km. Here, we use the term 'mean variations' to refer to results that are averaged over longitude and local time in a consistent manner. Previous results have been based on data from sun synchronous satellites, so that the local time at which the data are sampled are constant, and the zonal means are biased by that local time.

The results for both of these cases are new, and should provide added insight for understanding, and for comparing with theoretical results.

Our results are based on measurements from the Broadband Emission Radiometry (SABER) instrument (Russell et al., 1999) on the Thermosphere-Ionosphere-Mesosphere-Energetics and Dynamics (TIMED) satellite. SABER has now made global measurements nearly continuously since the beginning of 2002, and globally from ~20 km to over 100km, although our results are provided only for latitudes within 48° of the Equator. In addition, unlike almost all instruments on other satellites, SABER samples data over the range local solar time, and provide the potential to analyze quantitatively diurnal variations over 24 hrs of local time.

Our analysis here is based on previous results by us, using SABER data. References are given below. We are not aware of other comparable results for ozone from the stratosphere into the lower thermosphere, although there have been global results by others of temperature, as discussed below. Our previous results providing ozone and temperature values over the 24 hrs of local time and over the range of days over a year enable us to generate detailed correlation analysis between the two variables. We had already qualitatively noted this in Huang et al. [2008a, 2008b, 2010b] in relation the ozone and temperature quasi-biennial and semiannual oscillations.

As discussed below, the correlations between ozone and temperature for mean variations from day to day are more systematic, compared to that for diurnal variations over a daily cycle. For diurnal variations, the correlations show more varied patterns as a function of altitude, latitude. Both the ozone and temperature diurnal variations show systematic and regular phase progressions in local time, as a function of altitude and latitude. For temperature, these phase progressions represent migrating tides, and are expected. For day time ozone, we find regular phase progressions in local time over the whole altitude range of our analysis, 25 to 105 km, at least for low latitudes. This was not totally expected, although the ozone phase progression at lower altitudes had been noted by us and by others previously.

## **2.0 Saber data characteristics and analysis**

The following discussion has basically been presented previously in our papers (e.g., Huang et al., 2010a, 2010b, 2008a 2008b). We repeat portions here as a convenience to the reader.

SABER measurements provide the potential to estimate the variations of ozone as a function of local time over 24 hrs that data from other satellites generally do not provide. The SABER instrument (Russell et al., 1999) views the earth's limb to the side of the orbital plane (~74° inclination), and ozone emissions in the 9.6  $\mu\text{m}$  band are used to retrieve the mixing ratios, corresponding to the line-of-sight tangent point. Measurements are made over the globe from about 20 to over 100 km, over 24 hrs in local solar time, since the beginning of 2002. This kind of information has not been available previously, especially from one instrument. The level 2A data (version 1.07), provided by the SABER project, are interpolated to 4° latitude intervals and 2.5 km intervals, and for each day, averaged over longitude for analysis.

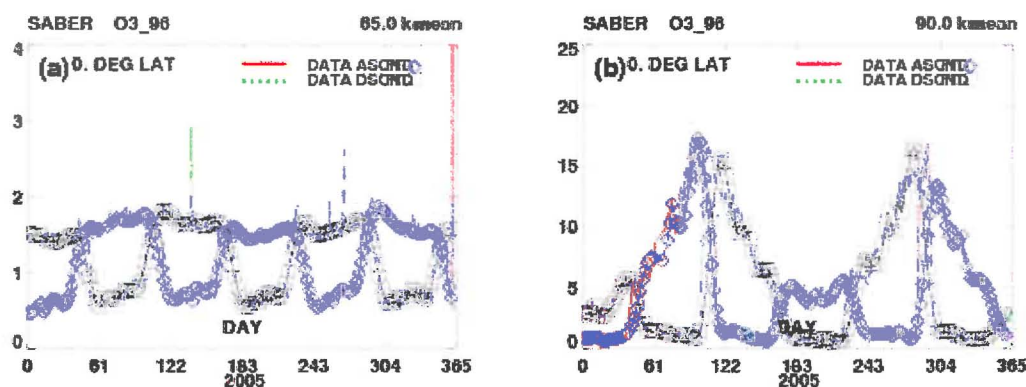
Over a given day and for a given latitude circle, measurements are made as the satellite travels northward (ascending mode) and again as the satellite travels southward (descending mode). Data at different longitudes are sampled over one day as the earth rotates relative to the orbit. The orbital characteristics of the satellite are such that over a given day, for a given latitude circle, and a given orbital mode (ascending or descending), the local time at which the data are measured are essentially the same, independent of longitude and time of day. For a given day, latitude, and altitude, we work with data averaged over longitude, one for the ascending orbital mode and one for the descending mode, each corresponding to a different local solar time, resulting in 2 data points for each day. Each can be biased by the local time variations, and is therefore not a true zonal mean. True zonal means are averages made at a specific time (not over a day) over longitude around a latitude circle, with the local solar time varying by 24 hrs over 360° in longitude. The local times of the SABER measurements decrease by about 12 minutes from day to day, and it takes 60 days to sample over the 24 hours of local time. Although this provides essential information over the range of local times, over 60 days, variations can be due to both local time and other variables, such as season. Diurnal and mean variations are embedded together in the data, and need to be unraveled from each other to obtain more accurate estimates of each. Therefore, although SABER data provide information as a function of local time that other satellites do not (the upper atmosphere research satellite, UARS is an exception), the measurements are still asynoptic, and there may be inherent limitations to the information content.

Our algorithm is designed for this type of sampling in local time, and provides estimates of both diurnal and mean (e.g., annual, semiannual oscillations) variations together in a consistent manner. It attempts to remove the bias in the mean due to the local time. As described in the Appendix, at a given latitude and altitude for data over a period of a year, the algorithm performs a least squares estimate of a two-dimensional Fourier series where the independent variables are local solar time and day of year, and variations as a function of local time and day of year over one year are generated. We currently do not generate results poleward of 48° latitude because data exist at the higher latitudes only on alternate yaw intervals (60 days). Because it takes SABER 60 days to sample over the range of local times, the sampling is less than ideal, and the information of the diurnal variations may be limited, and we limit the number of local time coefficients to 5. Once the coefficients are estimated, both the mean components (e.g., semiannual, annual, seasonal variations) and the diurnal variations can be calculated directly for any day of year. The algorithm has been applied previously to SABER ozone and temperature measurements to study diurnal variations and mean variations to study intra-seasonal (ISO), annual (AO), semiannual (SAO), and quasi-biennial (QBO) variations (Huang et al., 2006, 2006a, 2006b, 2008a, 2008b, 2010a, 2010b). It has also been successfully applied to wind measurements from the TIMED Doppler Interferometer (TIDI), as described in Huang et al., (2006a), and to the microwave limb sounder (MLS) on the Upper Atmosphere Research Satellite (UARS) ozone measurements (Huang et al., 1997).

Figure 1 shows an example of the sampling properties of SABER data and how well our algorithm estimates the data. SABER ozone mixing ratio data, averaged over longitude, at the Equator, 65km (left plot a) and 90 km (right plot), are plotted versus day for data from year 2005. For a given day, the solid red line and dashed green line represent the data from the ascending and descending modes, respectively, each corresponding to one local time. The two data points for each day can differ significantly from each other, reflecting different local times. The local times decrease by about 12 minutes from day to day. The blue diamonds and black squares represent our estimates, by evaluating the fit at the same day and local time as the data. As can be seen, the



estimates approximate the measurements reasonably, although there are some intervals over several days where our estimates do not follow the data as well, so some smoothing exists.



**Figure 1.** Zonally averaged SABER ozone data (ppmv) and estimated results plotted versus day of year based on data from 2005, at the Equator, 65 km (left plot, a) and 90 km (right plot, b). Solid red line and blue diamonds represent ascending mode data and fit, respectively. Dashed green line and black squares represent descending mode data and fit, respectively. The fits are evaluated at the same day and local time as the data.

### 3.0 Mean variations.

As noted earlier, we use the term ‘mean variations’ to denote the variation of ozone and temperature that are averaged over both longitude and local time in a consistent manner, as would be the case if the data were taken globally at one time, as in a snap shot, consistent with three-dimensional models. Again, we make this distinction because in previous empirical results by others, the averages are over longitude, but the measurements all represent one local time.

#### 3.1 Ozone and temperature mean variations derived from SABER measurements

For mean variations, we had previously derived from SABER zonal mean ozone and temperature measurements, from ~20km to 100km, and from 48°S to 48°N latitudes, since the beginning of 2002. In Huang et al. [2006] for temperature, and Huang et al. [2008a] for ozone, we had analyzed the results by considering the seasonal, semi-annual (SAO), annual (AO), and quasi biennial (QBO) oscillations.

Correlative studies of mean ozone and temperature variations are not new. However, previous studies have largely been limited to the stratosphere and lower mesosphere, and are based on data at one fixed local time. Here, we extend results into the mesosphere and lower thermosphere. In the next subsection, we extend the results to local time variations, which have not been available before.

#### 3.2 Correlations of ozone and temperature mean variations

For mean variations from day to day, Barnett et al. [1975] showed, using zonal mean data from the Nimbus 4 satellite (the back scatter ultraviolet spectrometer (BUV) and the selective chopper radiometer (SCR) instruments) that near 48 km altitude (~1 hPa), there is a general anti-correlation between ozone and temperature variations. This was consistent with their daytime chemical model, which showed that the dependence on temperature of ozone photochemical reaction-rates leads to



negative correlations over time. They also showed that in this altitude region, dynamical effects are not important.

Finger et al. [1995] analyzed ozone data from the Nimbus 7 Solar Backscatter Ultraviolet Radiometer (SBUV) and the temperature analysis from the National Centers for Environmental Prediction, Climate Prediction Center (NCEP/CPC) taken over more than a decade. Generally, they found an overall positive correlation between ozone and temperature in the lower stratosphere and a mostly negative correlation in the upper stratosphere. Chandra [1986] also analyzed Nimbus 7 ozone and temperature measurements between ~25 and 60 km. He found that the correlation between ozone and temperature shows a clear transition from positive to negative at all latitudes, with the zero correlation line varying from about 10 mbar (~32 km) at low latitudes to about 4 mbar (~35 km) at higher latitudes on the winter side. As indicated earlier, these and other studies based on satellite measurements involve data sampled at a fixed local time, and the results can be biased. However, because correlations deal with relative variations, the biases need not significantly affect the results.

However, Rood and Douglass [1985] and Douglass et al. [1985] show that dynamics can also cause significant anti-correlations between temperature and ozone, so the situation may not always be simple to interpret.

Figure 2 shows correlation coefficients between ozone mean mixing ratios and temperatures, based on SABER data (years 2004 through 2007 merged), on altitude-latitude coordinates, between 48°S and 48°N, over a one year period. In the left plot, the correlations are between zonal means which are also averages over local time, while the right plot depicts our zonal mean results that correspond to a fixed local time, namely 14 hrs local time. Our results in Figure 2 show that the correlation between ozone and temperature are generally positive below ~35 km, and are negatively correlated between ~35 km and 80 km, with some deviations at mid-latitudes and altitudes. The results in Figure 2 are generally consistent with previous studies in the stratosphere and lower mesosphere.

Above about 80 km, the positive correlation between ozone and temperature, although not unexpected, are to our knowledge, new. This positive correlation indicates that the variations are more dependent on dynamics than on photochemistry. In this region, atomic oxygen (O) becomes more abundant than ozone, and the chemical loss time scale for O is ~ 1 day at 80 km, and ~ 1 week at 100 km (Allen, 1984, Brasseur and Solomon 2005). Based on chemistry alone, above ~80 km, O should not exhibit significant diurnal variations since its life time exceeds a day. However, as discussed below when we study diurnal variations, O can display significant diurnal variations, due to transport.

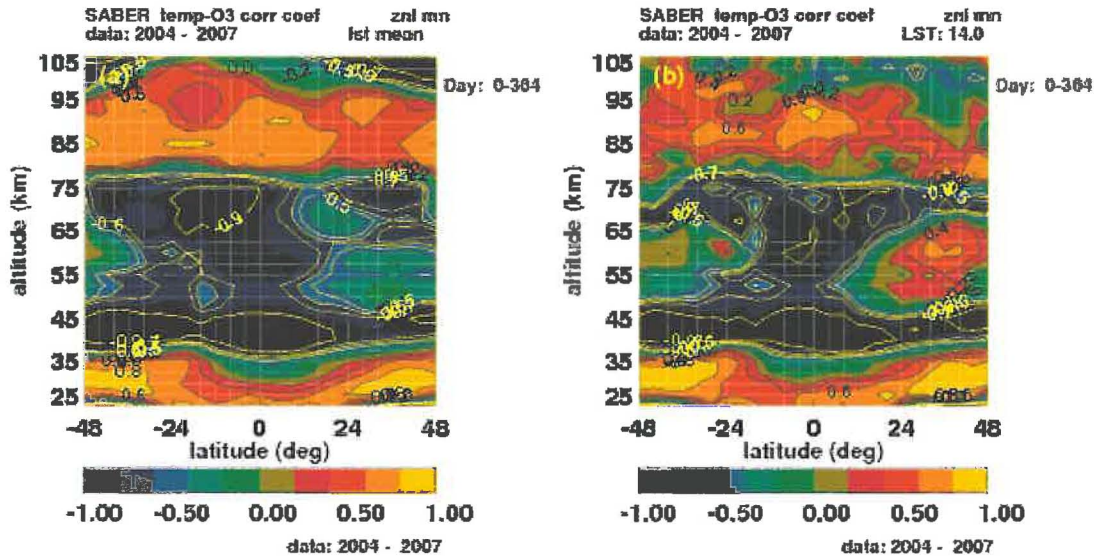
Figure 2 is also consistent with the model results of Garcia and Solomon [1985], who show that between about 30 and 80 km, odd oxygen,  $O_x$  ( $O + O_3$ ), is controlled more by photochemistry, while dynamics control regions below ~35 km and above ~80 km. Below ~ 25 km, the chemical lifetimes for odd oxygen are months or longer, due largely to attenuation of solar radiation.

Structurally, in Figure 2, the change in correlation from negative to positive near 80 km, at least for low latitudes, is due to the change in phase with altitude in the temperature. Although not shown, the temperature phases of the semiannual (SAO), quasi-biennial (QBO) and seasonal components change rapidly with altitude near 80 km, while the corresponding phases of ozone remains steady. In contrast, for the annual oscillation (AO), it is the phase of ozone, rather than that of the temperature, which changes with altitude near 80 km. Our temperature AO compares qualitatively well with the results by Remsberg et al. [2002], from ~32 to 80 km, based on data from the halogen occultation experiment (HALOE) on the upper atmosphere research satellite

(UARS). Although our amplitudes are generally larger, the morphology is quite similar. Remsberg et al., [2002] do not provide results above 80 km, nor any ozone results, so further comparisons are not made.

Similar results for the temperature SAO have been found by Garcia et al. [1997], based on data from the Solar Mesosphere Explorer (SME) satellite, and by Shepherd et al. [2004], based on WINDII data on UARS.

In contrast to the situation near 80 km, the change in sign of the correlation near 35 km is due to the change in the phases of ozone instead of the temperature. This behavior near 35 km is discussed further in Huang et al. [2008a].



**Figure 2.** Correlation coefficients between ozone zonal mean mixing ratios and temperatures over a one-year period, based on SABER data (years 2004 through 2007 merged), on altitude-latitude coordinates; a) left plot: results that are averaged over local time; b) right plot: results that are at 14 hrs local time.

#### 4.0 Diurnal variations

For diurnal variations over 24 hrs in local time, as with the mean variations, we had previously derived from SABER zonal mean ozone and temperature measurements, results from ~20km to 105km, and from 48°S to 48°N latitudes. See Huang et al. [2010a, 2010b, 2008b, 2006a, 2006b].

Here, we analyze the correlations globally over 24 hours of local time, and these results are new, as we are unaware of comparable results by others.

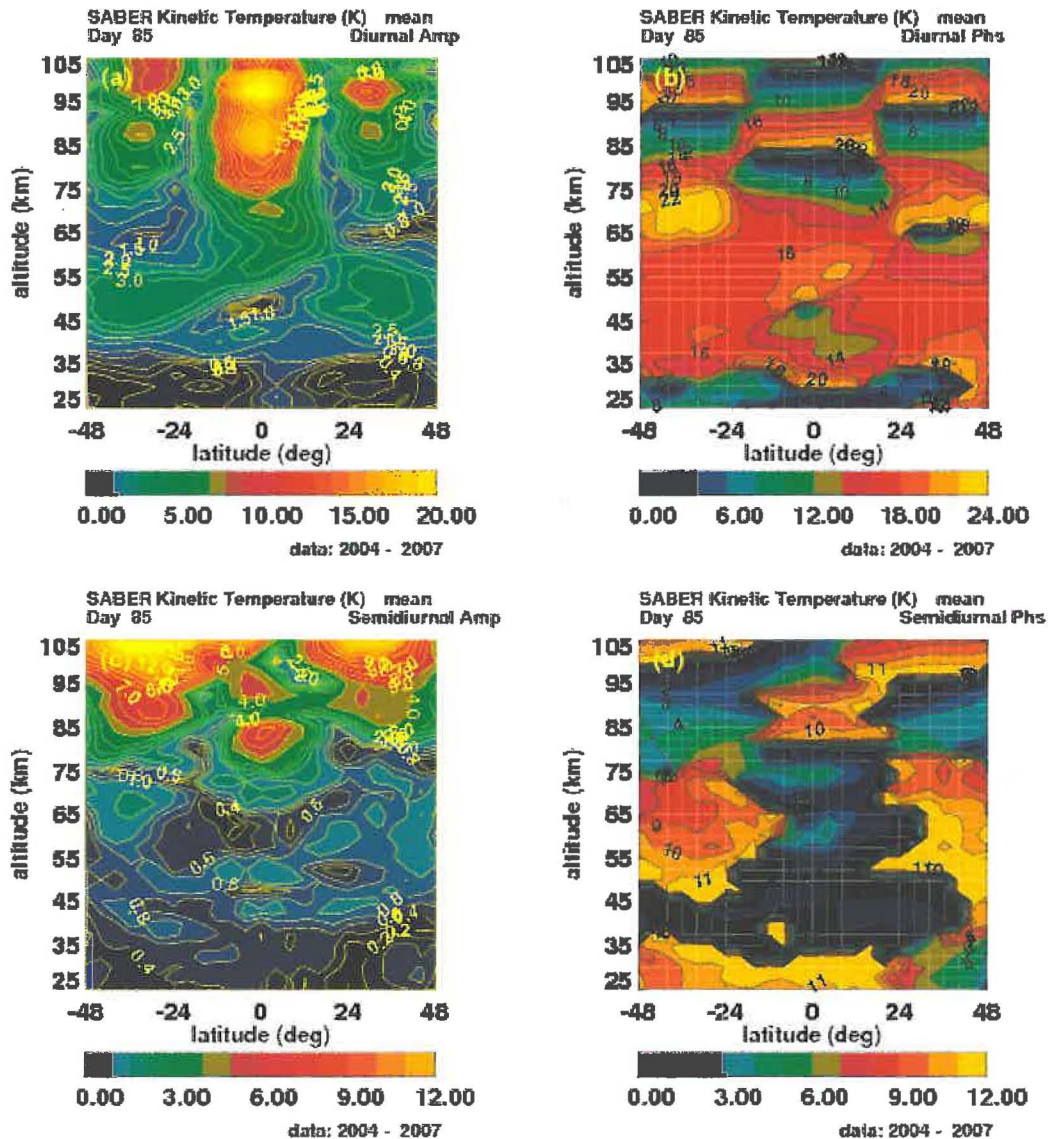
In Section 6 (Comparison of diurnal variations with other measurements), we compare with results by others using different data.

##### 4.1 Temperature diurnal variations based on SABER measurements

Because we use zonal means, and because of the sampling footprint of the SABER instrument in local time, the diurnal variations of temperature reflect thermal migrating tides, which are due to absorption of solar radiation by ozone and water vapor. Temperature diurnal variations have been studied empirically and theoretically much more than ozone diurnal variations, and we will but give a few references here (e.g., Chapman and Lindzen [1970], Forbes and Garret, [1979], Hagan et al., [1999], Mayr et al., [2005]).



Figure 3 (a, top left) shows the migrating tide diurnal amplitudes in altitude-latitude coordinates for day 85, based on SABER data from 2004 through 2007 merged together, from 25 to 105 km. It can be seen that near the equator, the diurnal amplitudes near 85 and 95 km contain local maxima, with secondary maxima near  $\pm 35^\circ$  latitude. The top right (b) plot of Figure 3 shows the corresponding phases. The expected propagating diurnal phase progression with altitude and latitude is evident near 60 km and above, consistent with the first symmetric propagating tidal mode. Note from Figure 3 (b) that the secondary maxima near  $\pm 35^\circ$  latitude are out of phase with the maxima at the equator. The bottom row corresponds to the top row, but for semidiurnal amplitudes and phases. We refer the reader to Huang et al. [2010a] for additional comparisons of our temperature results to those of others.



**Figure 3.** Top row: a) diurnal temperature (K) migrating tide amplitudes (left) and b) phases (hr of maximum) for day 85 based on data from 2004 through 2007 merged, from 48°S to 48°N latitude, 25 to 105 km; bottom row: as in top row, but for semidiurnal amplitudes and phases.



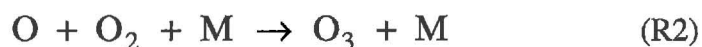
## 4.2 Ozone diurnal variations based on SABER measurements

Ozone diurnal variations are essentially due to photochemistry, the changing solar zenith angle over a day, and to transport dynamics. Unlike the case for mean variations, effects of dynamics in the form of tidal transport (which are averaged out for mean variations) can be significant, especially in the MLT. Over time scales of a day or less, the efficacy of ozone and temperature response to each other, and the dependency of photochemical reaction rates on temperature are added considerations.

Ozone mixing ratio diurnal variations generally become more prominent with increasing altitude from the stratosphere, abates on approaching ~80 km, after which the variations becomes largest between 80 and 100 km.

Figure 4 shows our derived zonal mean temperature (°K, left plots) and ozone mixing ratios (ppmv, right plots) versus local solar time, for day 85, at the Equator, from 50 to 80 km, based on SABER measurements for data from years 2004 through 2007, merged together. Figure 5 continues Figure 4 for altitudes from 80 to 100 km.

It can be seen that for ozone (right plots), the larger variations at the higher altitudes occur near sunrise and sunset, and are mostly the result of the relatively fast reactions



which represent the photolysis of ozone ( $\text{O}_3$ ) by solar radiation (R1) and the recombination of molecular ( $\text{O}_2$ ) and atomic ( $\text{O}$ ) oxygen back to ozone (R2), together with a third body, M. Molecular oxygen is relatively abundant, so the creation of ozone depends largely on the amount of available atomic oxygen and the amount of M. With decreasing altitude from the mesosphere on down into the stratosphere, the diurnal variations become less significant, as daytime ozone photolysis (R1) becomes slower and conversion back to ozone (R2) becomes faster, although other reactions (e.g., involving  $\text{NO}_x$ ,  $\text{ClO}_x$ ,  $\text{HO}_x$ ) also effect the variations of ozone over a day (see e.g., Allen et al., 1984; Vaughan, 1984, Pallister and Tuck, 1983, Brasseur and Solomon, 2005).

In the middle and lower stratosphere, the abundance of atomic oxygen is small compared to that of ozone, and the lifetime of ozone is greater than a day. Therefore, relatively small diurnal variations are expected to occur in the stratospheric ozone concentrations. In the mesosphere, atomic oxygen concentrations can be comparable to or greater than those of ozone so that at the beginning of the night the recombination reaction leads to increases in ozone, and just after sunrise, photolysis leads to ozone decreases.

In order to study the response times of ozone and temperature to each other for time scales of one day or less, Froidevaux et al., [1989] used a simplified daytime chemical model at mid-latitudes, with input temperature perturbations of various periods less than one day. They show that, for a given sine wave temperature perturbation, the resulting ozone variation can be phase-shifted, with the amount of shift depending on the relative magnitudes of the period of the given temperature perturbation compared to the ozone chemical relaxation time. Basically, for altitudes above ~48 km and temperature periods ~ 10 hrs, ozone and temperature could react efficiently to each other. So at these altitudes, the ozone and perturbation should be out of phase with the temperature, based on the dependence of photochemical reaction rates to temperature. Vaughan [1984] has also shown that the ozone can be sensitive to temperature changes over a diurnal cycle. Our results (not shown)

for the terdiurnal amplitudes show that they can be larger than 1°K (~70 km) and approach 5°K (between ~90 and 100km), so temperature perturbations with periods of 8 hrs can be significant at high altitudes.

As for effects of tidal transport, previous studies include those by Allen et al. [1984]; by Zommerfelds et al. [1989], based on ground based-radiometers; by Huang et al. [1997], based on MLS/UARS; by Kaufmann et al. [2003], based on CRISTA; by Marsh et al. [2002], based on HRDI, and by Smith et al. [2008], based on SABER.

As examples, Zommerfelds et al. [1989] suggest transport as the cause for the post-midnight increase in ozone; Marsh et al. [2002] noted dynamical signatures in their daytime results of ozone in the mesosphere, noting that there are indications of vertical advection of atomic oxygen by the solar diurnal tide; Kaufmann et al. [2003] suggest that the ozone equatorial maximum near 95 km is likely due to downward transport of atomic oxygen due to atmospheric tides, and the latitudinal distribution is also strongly biased by thermal tides. In Huang and Reber [2001], we had found that diurnal variations are significant in the stratosphere and lower mesosphere even for CH<sub>4</sub> and N<sub>2</sub>O, whose lifetimes are much longer than one day, suggesting that transport due to thermal tides can be important. Haefele et al. [2008] provide examples of diurnal variations of H<sub>2</sub>O.

In our lower altitudes of interest, the diurnal thermal tide amplitudes are smaller, with temperature amplitudes up to ~ 5K at 55 km (~0.46 hPa), and decreasing to ~1K or less near 40 km (~4.6 hPa) and lower, as described in Huang et al. [2010a]. At even lower altitudes, our results show significant ozone diurnal variations at altitudes as low as ~25 km (~31 hPa), where photochemical effects are expected to be minimal.

At higher altitudes such as 95 km, near the equator, and equinox, Smith et al. [2008] used the SABER measurements of temperature and hydrogen to consider both dynamic and photochemical effects to determine the ozone diurnal variation. Because they consider only night versus day ozone values instead of variations over 24 hrs in local time, their variations appear symmetric with respect to midnight. Their ozone and temperature peak-to-peak values compare well with ours, considering that our results also contain semidiurnal and terdiurnal components, which, for temperature, can each be several °K at high altitudes. See Figure 5, bottom left (c) and right (d).

Because Smith et al. [2008] provide results for but one instance, where the tidal temperatures are out of phase in local time relative to ozone, it would be interesting if corresponding calculations are made at the same altitude, but at mid latitudes, where the ozone and temperature are more in phase with each other. This could give further support for their results. The different phase relationship at mid latitudes is due to the phase reversal of the tidal temperatures at mid latitudes relative to that near the equator, as discussed earlier in reference to Figure 3, and discussed below in Figure 8, concerning the ozone-temperature correlation.

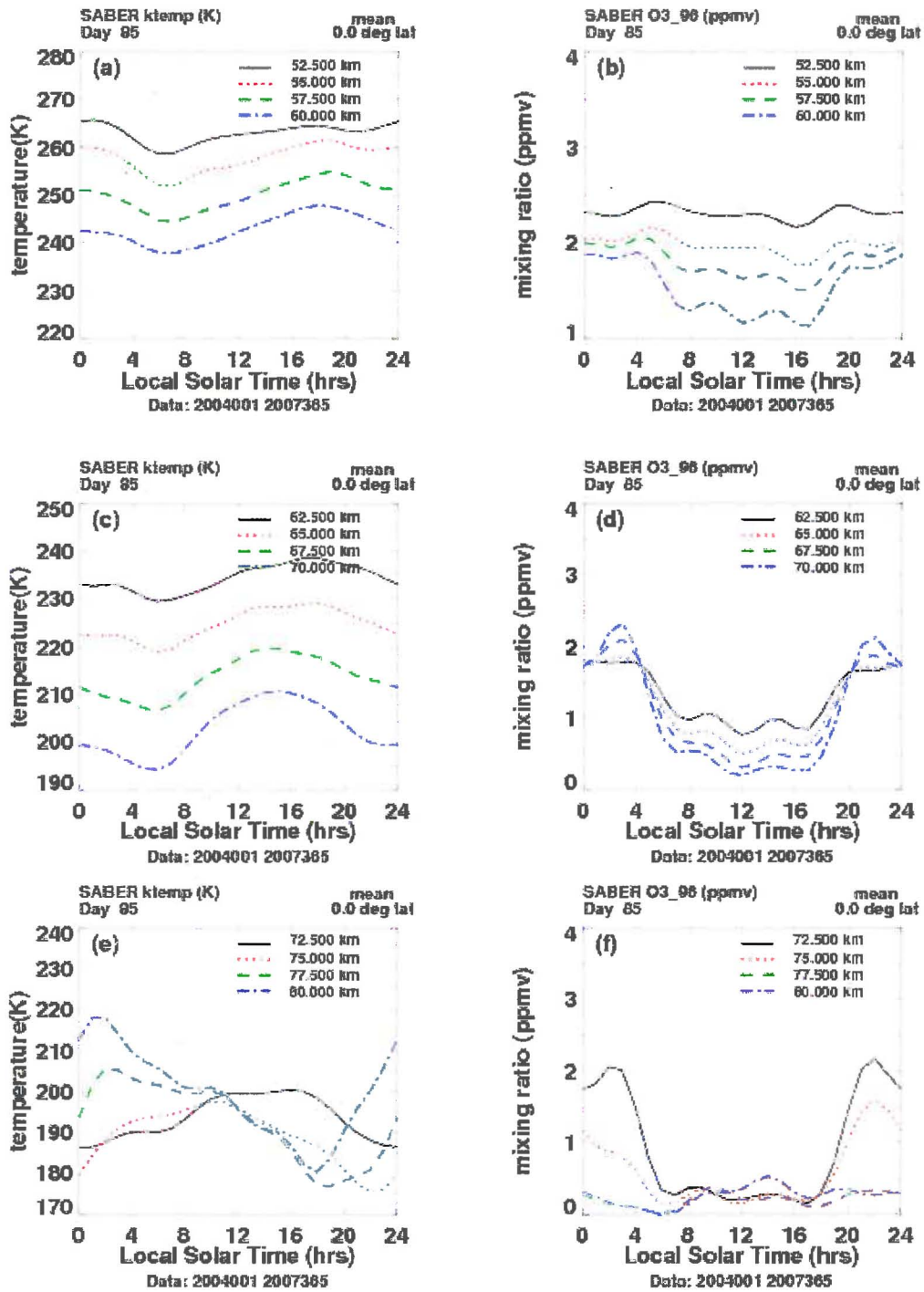
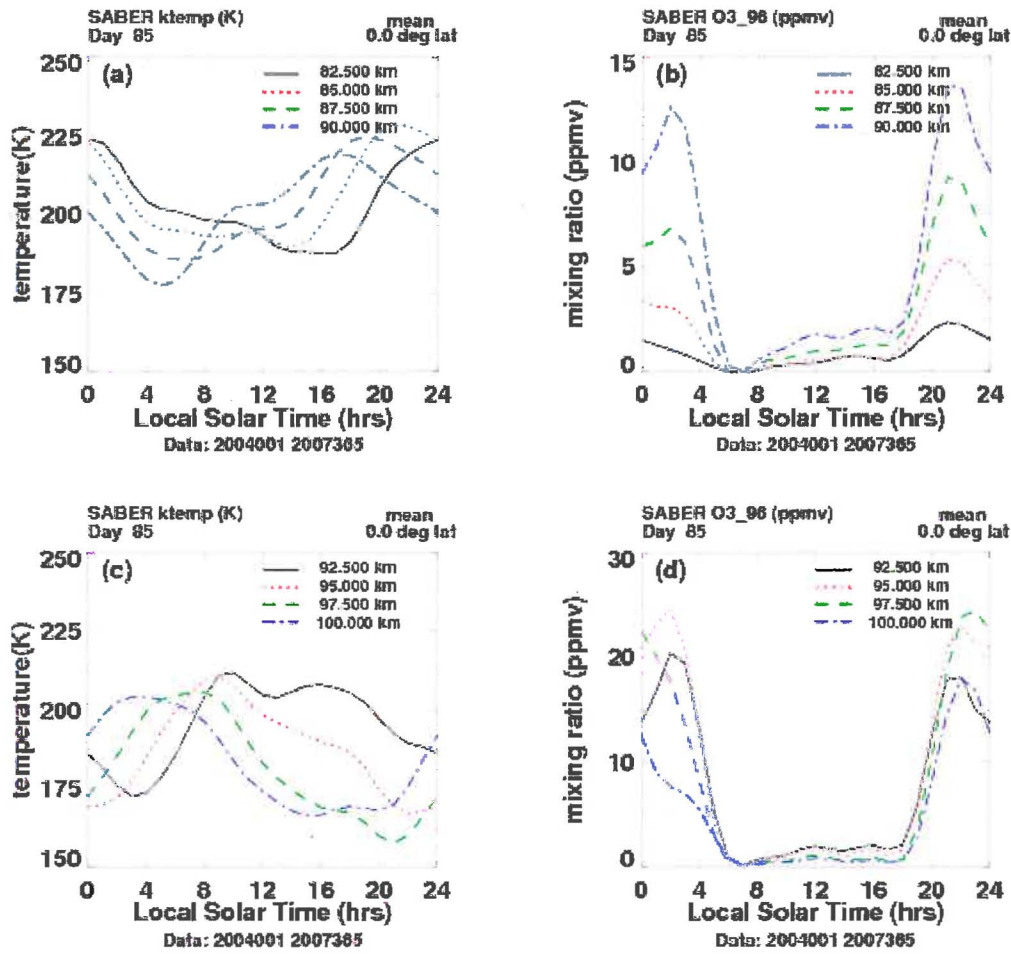


Figure 4. Derived diurnal variations of temperature (left plots) and ozone (right plots) based on SABER data (years 2004-2007), temperature (left plots) and ozone (ppmv, right plots) versus local time, from 50 to 80 km, at the Equator.





**Figure 5.** Derived diurnal variations of temperature (left plots) and ozone (right plots) based on SABER data (years 2004-2007), temperature (left plots) and ozone (ppmv, right plots) versus local time, from 82.5 to 100 km, at the Equator.

### 5.0 Ozone and temperature daytime phase progression and variation.

As noted earlier in reference to Figure 3, the temperature migrating tide shows phase progressions in local time as a function of altitude, especially evident above 60 km, as exemplified in Figure 3 (b) for the propagating diurnal component.

For ozone, because variations at the higher altitudes are mostly dominated by the changes near sunrise and sunset, and the photochemistry is different for day and night, here we focus on the daytime behavior, from 6 to 18 hrs. As with the temperature, for daytime ozone values, and low latitudes at least, there are systematic local time phase progressions as a function of altitude. For altitudes between 25 and 55 km, the phase progression is discussed in Huang et al. [2010b], and can be seen in Figure 7, which appears later in Section 6 and shows results at 40°N latitude for comparison with results done by others. The left plot (a) of Figure 7 shows the ozone mixing ratio plots versus local time from 25 to 55 km at 4, and is shown as a reminder of the relatively small magnitudes of the variations. The right plot (b) is the same as the left plot, but with the values being percent deviation from midnight, in order to display the small variations of a few percent more clearly. It shows that, as a function of altitude, the ozone diurnal variations show a pattern of

phase progression in local time, such that beginning at ~25 km (~31 hPa) to higher altitudes, the mixing ratios become mostly larger in the afternoon. As the altitude increases, the afternoon values grow relative to their mean values, so that near ~40 km (~2.1 hPa), the mixing ratios in the afternoon are mostly larger than to the values earlier in the day. As the altitude continues to increase to near 55 km (~0.46 hPa), the afternoon values again become mostly smaller than values earlier in the day. As discussed in Huang et al. [2010b], this pattern is supported by measurements from the microwave limb sounder (MLS) on UARS. It is also consistent with results from ground-based microwave measurements [e.g., Connor et al., 1994; Haefele et al., 2008] and chemical models (e.g., Pallister and Tuck, 1983, Huang et al., 1997).

As the altitude continues above 55 km, these progressions can be seen in Figures 4 and 5 that this latest trend for daytime continues (i.e., ever decreasing daytime values) to higher altitudes in the mesosphere, at least for low latitudes.

However, starting at ~ 75 km, for the ozone daytime behavior, this trend is reversed, and with ever increasing altitude, the afternoon values again become larger, as can be seen in Figure 4 (f, bottom row, right). Figure 5 (right plots) shows that this last pattern of larger late afternoon values continues to near 90 km, after which near 100 km, the afternoon values again become comparable to values earlier in the day.

From 70 to 82.5 km, our results are in qualitative agreement with those of Marsh et al. [2002], alluded to earlier, including the shift of larger values to later in the afternoon. Marsh et al. [2002] attribute this behavior in part to water vapor and odd-hydrogen chemistry, and a delay in ozone destruction, referring to Vaughan [1984]. Marsh et al. [2002] do not provide results at other altitudes, and we cannot compare further.

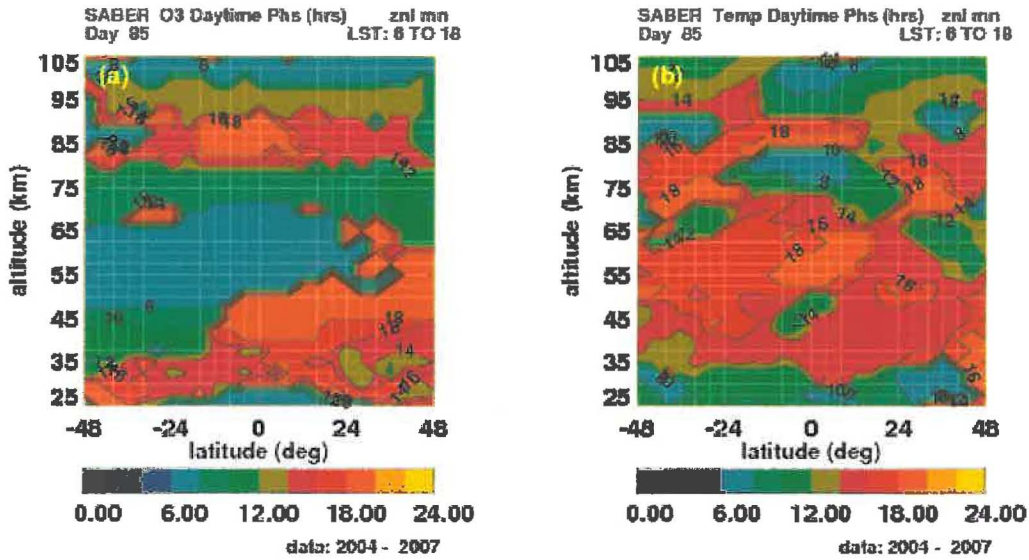
In summary, for low latitudes, the altitudes at which ozone diurnal variations maximize later in the afternoon are near 45 km and 90 km. The altitudes at which ozone are generally minimal in the afternoon corresponds to ~25 km, 70, and 100 km. The altitudes at which the temperature diurnal variations maximize later in the afternoon are ~ 45, 70, and 90 km, and the corresponding altitudes for temperature minima in afternoon are ~25, 45, 80, 100 km. Note that near 45 km, the temperature variations appear to support both maxima and minima in the afternoon. The reason is that near 45 km, the temperature phase progression reverses as the altitude increases.

What is new here is that, for ozone, the daytime phase progressions in local time are systematic, over the range from 25 to at least 100 km, near the upper limit of our study, although the progression at lower altitudes had been noted in previous studies.

For other latitudes, this phase progression just described can be seen in Figure 6, which shows derived daytime (6 to 18 hrs) phases (hr of max value) for ozone (left plot) and temperature (right plot), on altitude-latitude coordinates (25 to 105 km, 48°S to 48°N), based on SABER data from 2004 through 2007 merged together. As can be seen, the temperature phases retain much of the morphology of the diurnal tide shown in Figure 3 (b, top right), retaining not only the phase progressions as a function of altitude, but also the symmetric phase changes in local time, with respect to the equator, in particular above 60 km, typical of the migrating tide. Note however, that in Figure 6, the phase is for the temperature itself, while Figure 3b reflects the phase of the diurnal component only.

For ozone, at the higher altitudes above 60 km, although the ozone phases continue to change with altitude, they do not exhibit the phase changes with latitude that the temperatures do.

This obviously has significant effects on the correlations between ozone and temperature, as discussed below in Section 7.



**Figure 6.** Daytime (6 to 18 hrs) phases (hr of max value) for ozone (left plot) and temperature, on altitude-latitude coordinates (25 to 105 km, within 48° of equator), based on SABER data from 2004 through 2007 merged together.

## 6.0 Comparison of diurnal variations with other measurements

Because some of the variations in Figures 4 and 5 can be relatively small, especially for ozone, we summarize some previous analyses of our results and comparisons with other measurements, given in Huang et al. [2008b, 2010b] for ozone, and in Huang et al. [2010a] for temperature.

For ozone, outside of our previous results, there are scant comparable (global, temporal coverage) studies for variations over a diurnal cycle with which to compare. Mostly, results by others are generally at fixed locations and at selected altitudes, so we can only make spot comparisons. These include data from ground-based microwave techniques, on rocket-borne photometers, and MLS and HRDI on UARS.

Our comparisons focus not on absolute values, but on relative variations, as these are pertinent to our analysis. The comparisons show good qualitative agreement.

The left plot (a) of Figure 7 shows the ozone mixing ratio plots versus local time from 25 to 55 km at 40°N latitude, which is closer in location to that of some other measurements, and is shown as a reminder of the relatively small magnitudes of the variations. The right plot (b) is the same as the left plot, but with the values being percent deviation from midnight, in order to display the small variations more clearly.

At 55 km (~0.46 hPa), our results in Figure 7 show local maxima near 6, 14, and 19 hrs. The results of Ricaud et al. [1996], based on MLS UARS, of Haefele et al. [2008] and Connor et al. [1994], based on ground-based radiometers, are all consistent with our results. All show local peaks near 6 and 18 hrs, and local maxima near 14 hrs. Results from Lean [1982], based on rocket-borne photometer data, also show the local maxima in the afternoon (variations before 6 and after 18 hrs are not provided by Lean). The UKMO chemical model also shows the local maxima at 0.46 hPa.

These local maxima also show a smooth transition to higher altitudes in the mesosphere, where the results also show one or more daytime local maxima [Huang et al., 2008b], and are consistent with results from Marsh et al. [2002], who provide daytime results of ozone from 70 to 82.5 km, based on measurements from HRDI on UARS, noted above. Their results are also consistent with



the phase progression in local time that we find, as discussed earlier in Section 5 (Ozone and temperature daytime phase progression and variation).

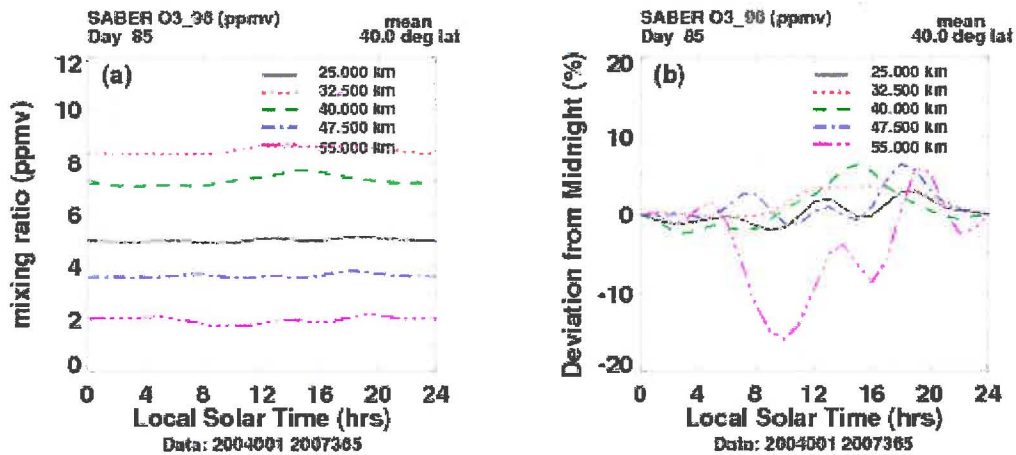
Near ~39 km (~3.1 hPa) and mid latitudes, our results are again consistent with those of Haefele et al. [2008], Connor et al. [1994], and Lean [1982]. There is also good qualitative agreement with results from both MLS UARS over a range of altitudes. For example, the variations at 40 km in Figure 7 show a maximum of about 5 percent near 16 hrs. This compares well with corresponding results by Haefele et al. [2008]. In addition, the ground-based results by Haefele et al. [2008] at ~25 km (~27 hPa) also agree well with our results at 25 km and with the chemical model of Herman [1979] near 30 km.

Considering that the results of ground-based radiometers are averaged over days or longer, and have a relatively coarse altitude resolution, the agreement is qualitatively quite good.

Again, for more details, we refer the reader to Huang et al. [2010b, 2008b] for ozone.

For temperature diurnal variations, we refer to Huang et al. [2010a, 2006b, 2006a]. In addition to our derived results for temperature, there have been those by others (e.g., Zhang et al. [2006], Xu et al. [2007], and Mukhtarov et al. [2009]) who have generated comparable results, also based on SABER data, and which compare quite well with ours. For example, Mukhtarov et al. [2009] have generated diurnal amplitudes at 75 and 95 km, and they report that differences between their values and ours are ~ 1°K or less.

As noted earlier, we had also derived results of the SAO and QBO for ozone and temperature. These too, have been compared with other measurements, and qualitatively, the comparisons are quite good. For ozone, we refer to Huang et al. [2008a], and for temperatures, to Huang et al. [2006]. The good comparison for the SAO and QBO are also pertinent to the quality of the diurnal variations due to the manner which our results are obtained. As discussed earlier, both diurnal and variations mean variations (e.g., SAO, QBO) are embedded together in the data, and need to be unraveled from each other to obtain more accurate estimates of each. From the mathematical view, the diurnal and mean variations in the data are on equal footing, and obtaining robust estimates for the one reflects on that for the other, as our algorithm estimates these variations together.



**Figure 7.** a) Ozone mixing ratios versus local time at 40°N, from 25 to 55 km; b) as in a) but for percent deviation from midnight, to show small variations more clearly.

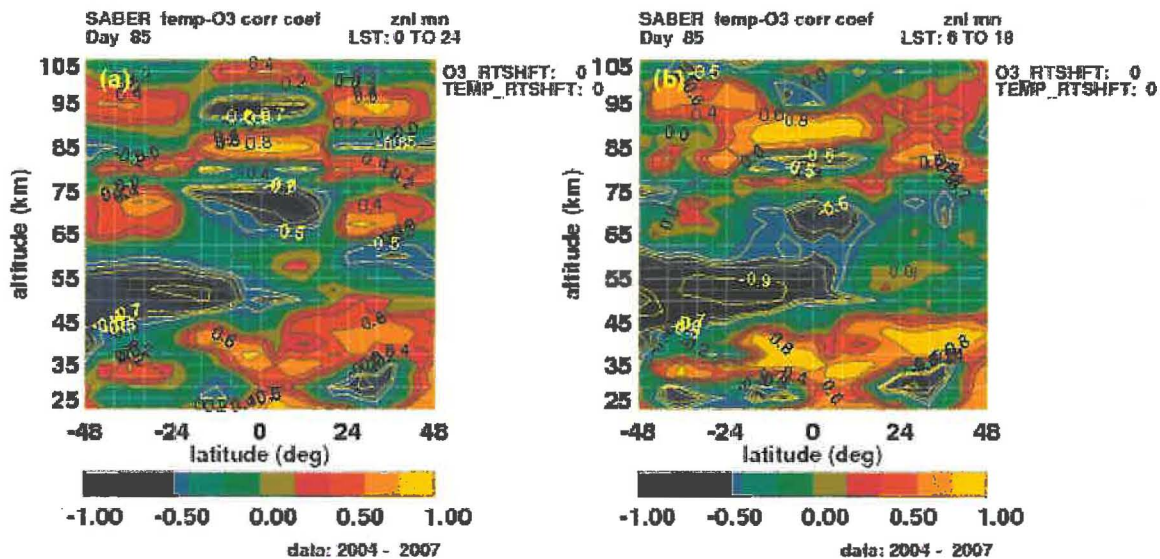
## 7.0 Correlations of ozone and temperature diurnal variations

Figures 4 and 5 show in detail the ozone and temperature variations at the equator and Figure 6 indicates similar variations at other latitudes, including the progression in local time phase as a function of altitude. Figure 6 also provides an indication of the nature of relative ozone and temperature diurnal variations to each other.

Figure 8 shows the correlation coefficients between ozone and temperature for day 85, on altitude versus latitude coordinates, from 25 to 105 km within 48° of the Equator. The left plot (a) shows correlations over 24 hrs local time, while the right plot (b) shows correlations over day time (6 to 18 hrs) only. Although the over-all patterns appear similar between the left and right plots, at higher altitudes, the pattern appears to be slightly shifted in altitude, between the plots.

As can be seen, the correlations are less systematic compared to the corresponding correlations for mean variations shown in Figure 2, especially at higher altitudes. Up to ~40km, the correlations are mostly positive/neutral, while that from 40 to 65 km are mostly negative/neutral. Because of indications of some similarity compared to the correlations in the mean variations seen in Figure 2 in this region, it suggests that both photochemistry and transport effects by tides need to be considered.

From ~65 to 105 km, the correlations can be negative or positive depending on the latitude and altitude. This pattern appears to reflect the phase plot of the temperature diurnal tide in Figure 3(b), and is reminiscent of the first symmetric propagating tidal mode, including the secondary maxima at mid latitudes (e.g., near  $\pm 35^\circ$ ) that are out of phase with the maxima at the equator. This can also be seen qualitatively in Figure 6, which displays the local time phases of ozone and temperature only for day time variations. The pattern seen in Figure 8 above ~65 km are in large part because the ozone variations do not show the same reversal in local time phase with latitude that the temperatures do, and the correlation coefficients in Figure 8 reflect this difference between ozone and temperature.



**Figure 8.** a) Correlation coefficient between ozone mixing ratios and temperatures on altitude-latitude coordinates, from 25 to 105 km, 48°S to 48°N, day 85 based on SABER measurements for years 2004 through 2007 merged; b) as in a) but only for daytime (6 to 18 hrs ).

## 8.0 Summary and discussion

We have analyzed the derived ozone and temperature variations based on measurements from the SABER instrument on TIMED. The variations include zonal mean diurnal variations over 24 hrs in local time and mean variations that are averaged over local time. The results are based on data from 2004 through 2007, from altitudes from 25 to 105 km, within 48° of the equator.

Because the variations, especially daytime ozone, can be small, we have reviewed comparisons made with other measurements, and they are all qualitatively consistent.

For mean variations, we have extended previous correlative studies to the upper mesosphere and lower thermosphere. Consistent with previous studies in the stratosphere and lower mesosphere, our results show that the correlations over 365 days between ozone and temperature are generally positive below ~35 km, and negative between ~35 km and 80 km, with some deviations at mid-latitudes and altitudes. They are also consistent with the view that where photochemistry is more in control, the correlations should be negative, due to the dependence of photochemical reaction rates temperature. Above about 80 km, we find mostly positive correlations between ozone and temperature, and although not unexpected, they have not been heretofore available. This positive correlation indicates that the variations are more dependent on dynamics than on photochemistry. Structurally, the change in correlation from negative to positive near 80 km, at least for low latitudes, is due to the change in phases with altitude in the temperature. In contrast, near 35km, the change in sign of the correlation is due to the change in the phases of ozone instead of the temperature.

For diurnal variations over 24 hrs in local time, the correlation results are new. The daytime ozone and temperature both display phase progressions in local time as a function of altitude from 25 to 105 km. For the temperature diurnal variation, the phase progressions was as expected, while that for ozone over the range from 25 to 105 km altitude were not expected, although in previous studies, the progression was noted for lower altitudes. The ozone-temperature correlations over a diurnal cycle are less systematic compared to that for mean variations. Up to ~40km, the correlations are mostly positive/neutral, while that from 40 to 65 km are mostly negative/neutral, and there are some similarities with the corresponding situation for the mean variations, suggesting that both photochemistry and transport effects by tides need to be considered. From ~65 to 105 km, the correlations can be negative or positive depending on the latitude and altitude. This pattern qualitatively reflects that of the temperature diurnal tide, including the secondary maxima at mid latitudes that are out of phase with the maxima at the equator. The correlation pattern above ~65 km is in large part because the ozone variations do not show the same reversal in local time phase as a function of latitude that the temperatures show.



## Appendix

### Data Analysis Algorithm

For a given latitude and altitude, the algorithm performs a two-dimensional Fourier least squares analysis in the form

$$\Psi(t_1, d, z, \theta, \lambda) = \sum_n \sum_k b_{nk}(z, \theta, \lambda) e^{i2\pi n t_1} e^{i2\pi k d / N} \quad (1)$$

where  $\Psi(t_1, d, z, \theta, \lambda)$  represents the input data;  $z$  is altitude;  $d$  is day of year;  $\theta$  latitude;  $\lambda$  longitude (radians);  $t_1$  = local solar time (fraction of a day) =  $t + \lambda / 2\pi$ ;  $t$  = time of day (fraction of day), and  $N$  is the number of days in the fundamental period. For example, if we analyze data over one year, then  $N = 365$ .

In this study, we apply the algorithm to data averaged over longitude, although it has been applied to data with longitude variations as well (Huang and Reber, 2004). For variations with longitude, we use data at discrete longitudes  $\{\lambda_i\}$  to find the set  $b_{nk}(z, \theta, \lambda_i)$  from (1). To analyze the behavior with longitude, we estimate  $\alpha_{mnk}(z, \theta)$  from

$$b_{nk}(z, \theta, \lambda_i) = \sum_m \alpha_{mnk}(z, \theta) e^{i2\pi m \lambda_i / 2\pi} \quad (2)$$

again using a least squares fit. Finally, for any day of year  $d_0$ , we can sum (1) over  $k$  to obtain

$$\Psi(t, d_0, z, \theta, \lambda) = \sum_m \sum_n \beta_{nm}(z, \theta) e^{i2\pi m \lambda / 2\pi} e^{i2\pi n t} \quad (3)$$

where we use  $\beta_{nm}$  to denote the transform to universal time  $t$  (fraction of a day).

If we average the data over longitude, then we obtain the migrating diurnal variations and mean flows (Huang and Reber, 2003) from (1), where the coefficients are no longer dependent on  $\lambda$ . Once we have estimated the coefficients in (1) or (3), we can directly generate the diurnal variations for composition, winds, and temperature as a function of day of year, longitude, and time. TIMED sampling patterns are such that data at latitudes poleward of about  $50^\circ$  are made only for alternate yaw periods. Therefore, our current analyses are made only within  $48^\circ$  of the Equator. Our fits to the data are based on data over a period of one year or more. Currently in (1), the maximum value of  $n$  is 5 for ozone, and the maximum of  $k$  depends on the fundamental period in day of year. Because it takes SABER 60 days to sample over the range of local times, when the fundamental day-of-year period is 365 days, we estimate the coefficients  $b_{nk}(z, \theta, \lambda_i)$  for  $k$  greater than or equal to 3 only for  $n = 0$ , and the maximum of  $k$  is 6. When the fundamental period corresponds to the QBO, the number of terms for day-of-year is scaled up accordingly. The current version of the data does not provide for uncertainties, and we also assume that the uncertainties of the data are proportional to the data values themselves.

### Acknowledgments:

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